Overview of the entropy production of incompressible and compressible fluid dynamics

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Abstract In this paper, we present an overview of the entropy production in fluid dynamics in a systematic way. First of all, we clarify a rigorous derivation of the incompressible limit for the Navier-Stokes-Fourier system of equations based on the asymptotic analysis, which is a very well known mathematical technique used to derive macroscopic limits of kinetic equations (Chapman-Enskog expansion and Hilbert expansion are popular methodologies). This allows to overcome the theoretical limits of assuming that the material derivative of the density simply vanishes. Moreover, we show that the fundamental Gibbs relation in classical thermodynamics can be applied to non-equilibrium flows for generalizing the entropy and for expressing the second law of thermodynamics in case of both incompressible and compressible flows. This is consistent with the Thermodynamics of Irreversible Processes (TIP) and it is an essential condition for the design and optimization of fluid flow devices. Summarizing a theoretical framework valid at different regimes (both incompressible and compressible) sheds light on entropy production in fluid mechanics, with broad implications in applied mechanics.

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1 Introduction and motivation

Entropy is a fundamental concept in both physics and engineering. It plays a prominent role in thermodynamics, statistical mechanics, continuum physics, information theory and, more recently, also in biology, sociology and economics. More details about the broad spectrum of involved disciplines can be found in Ref. [1] (and references therein) and some historical notes in Ref. [2]. One of the reasons of the fascination that scientists have always felt with regards to entropy is due to the fact this concept is one of the few (maybe the only one) dealing with irreversibility, the arrow of time and, ultimately, the evolution of life. As an example, to this respect we notice that recently the evolutionary strategy of cave spiders has been interpreted by means of an entropic argument [3]. In fact, most of the quantum equations of motion are time-reversible (with few exceptions, see [4]), as pointed out by the Loschmidt's paradox which is still source of discussions nowadays (partially solved by the fluctuation-dissipation theorems, see next). The term entropy was introduced in 1865 by the German physicist Rudolf Clausius. The idea was inspired by an earlier formulation by Sadi Carnot of what is now known as the second law of thermodynamics. The Austrian physicist Ludwig Boltzmann and the American scientist Willard Gibbs put entropy into the probabilistic framework of statistical mechanics (around 1875). This idea was later developed by Max Planck. Entropy was extended to quantum me-

chanics in 1932 by John von Neumann. Later this led to the invention of entropy as a term in probability theory by Claude Shannon (1948), popularized in a joint book with Warren Weaver, that provided foundations for information theory. The concept of entropy in dynamical systems was introduced by Andrei Kolmogorov and more deeply formulated by Yakov Sinai in what is now known as the Kolmogorov-Sinai entropy. The formulation of Maxwell's paradox (by James C. Maxwell, around 1871) started a search for the physical meaning of information, which resulted in the finding by Rolf Landauer (1961) of the heat equivalent for the erasure of one bit of information, which brought the notions of entropy in thermodynamics and information theory together. References for the above historical overview can be found in [1]. Remarkably, entropy is experiencing a new revival in computational science, driven by the recent developments in quantum computing (e.g. see [5]).

Many attempts have been made in order to rationalize the concept of entropy and its application to the second law of thermodynamics (e.g. see the efforts by Jakob Yngvason [6]). Beyond the axiomatic approach, the interpretation of entropy based on statistical mechanics still remains the most popular one [7]. Here, in particular, we focus on some fundamental results, with broad practical applications, obtained in the attempt to rationalize the physical meaning of irreversibility and entropy production. We present two examples: The fluctuation theorems and the mesoscopic numerical methods. Concerning the first implication (fluctuation theorems) studies in this context have been carried out over the past 15 years, and have led to fundamental breakthroughs in our understanding of how irreversibility emerges from reversible dynamics [8]. In 1993 Evans, Cohen and Morriss [10] considered the fluctuations of the entropy production rate in a shearing fluid, and proposed the so called Fluctuation Relation. This pioneering work has experienced an extensive development by different authors (see Ref. [11] and references therein). The original result has been extended to many different cases and it is now a whole new theoretical framework which encompasses the previous linear response theory and goes beyond that, to include far from equilibrium phenomena, such as turbulence and the dynamics of granular materials [11]. These results might have important implications also from the computational point of view. Indeed, these theorems aim at quantifying microscopic forces and understand how a system responds to external perturbations, using techniques such as molecular dynamics simulations [8]. Molecular dynamics simulations are powerful tools, even though the macroscopic interpretation of molecular results is far from obvious [9].

Enhancing our understanding about entropy production may have an impact beyond molecular simulations. An example is given by some trends in the mesoscopic numerical methods. In particular, the lattice Boltzmann method [12–16] is a powerful numerical method applied much beyond rarefied flows, including thermal radiation [17], thermal conduction [18], combustion [19–22], porous media [23,24], multi-component flows [25,26] and turbulence [27], to mention a few. Pertinently to this paper, the entropic lattice Boltzmann method was invented by Ilya Karlin and co-workers in 1998, by applying the maximum entropy principle to lattice kinetic equations [28]. Hence, the concept of entropy production boosted a tremendous development of further refinements [29–31]. A more complete review about the original development of entropic lattice Boltzmann method for hydrodynamic simulations can be found in Ref. [32]. Also in the case of numerical schemes for fluid dynamics, the entropy can be used as a design tool for generalizing the local equilibrium to include hydrodynamic moments beyond the conserved ones [33]. This allows one to design novel collisional kernels with improved stability [34]. Moreover, entropy may give a systematic guideline to derive advanced lattices by factorization symmetry [35], and it also reveals a key notion in dissipative dynamical systems for discerning between fast and slow processes [36–41].

In spite of the broad implications of entropy production (both in terms of fundamental theorems and practical numerical tools), its rigorous derivation in fluid dynamics for generic hydrodynamic regimes deserves a more detailed analysis. The need to clarify such elementary issues in the fluid dynamics community should not be a surprise [9]. The mathematical theory of fluids is in a very primitive state and the fluid dynamic equations do not have a fundamental nature [42]. Based on the former theoretical framework proposed by Lars Onsager, the pioneering idea by Ilya Prigogine to extend the fundamental Gibbs relation also to non-equilibrium states paved the way to the Thermodynamics of Irreversible Processes (TIP) [43,44]. The previous straightforward extension is based on the assumption of local equilibrium, i.e. all subparts of the system are close enough to equilibrium condition to be still described by classical thermodynamic variables and relationships. On the other hand, the Extended Irreversible Thermodynamics (EIT) [45,46] is an active field of research, where scientists make an effort to overcome the current limitations of the local equilibrium assumption. The basic idea is that thermodynamic quantities (e.g. entropy) depend also on dissipative fluxes (e.g. fluid

velocity) which are regarded as independent variables. The differential form of the generalized entropy leads to the generalized Gibbs relation for non-equilibrium states. Any non-equilibrium Gibbs relation should be considered as an assumption which satisfies the following requirements: i) it is Galilean invariant; 2) it reduces to the equilibrium Gibbs relation in the limit of quasi-static processes; 3) the conclusions derived from it are not contradictory and agree with experiments [47]. An example of the above procedure for studying non-equilibrium interfaces can be found in Refs. [48–50].

Compressible fluid dynamics has paid little attention to investigate entropy production (with very few exceptions, see Ref. [51]). Compressible fluid dynamics deals with flows having significant changes in fluid density. Significant compressibility occurs if the Mach number, which is the ratio between the characteristic speed and the local sound speed, is greater than about 0.2 [52,53]. The range of applications of compressible fluid dynamics includes aircrafts, spacecrafts (for re-entry), turbo-machinery and hypersonic plasmas. Compressible flows are usually characterized by shocks, i.e. an abrupt discontinuity in the flow field. Entropy condition (e.g. by Lax) is the typical admissibility condition used to discriminate the unique single-valued physical solution. Hence entropy is part of the state-of-the-art numerics for solving compressible flows [54]. However, in spite of this, little attention has been paid to rigorous entropy production in compressible flows, which could be helpful in guiding design and optimizations, as already happens in similar fields [55,56].

This paper aims to present an overview of the entropy production in fluid dynamics in a more systematic way. First of all, we present a rigorous derivation of the incompressible limit for the Navier-Stokes-Fourier system of equations based on the asymptotic analysis, which is a very well known mathematical technique used to derive macroscopic limits of kinetic equations (Chapman-Enskog expansion and Hilbert expansion are popular methodologies). This allows to overcome the theoretical limits of assuming that the material derivative of the density simply vanishes. Moreover, we show that the fundamental Gibbs relation in classical thermodynamics can be applied to non-equilibrium flows for generalizing the entropy and for expressing the second law of thermodynamics in case of both incompressible and compressible flows. This is consistent with the Thermodynamics of Irreversible Processes (TIP) and it is an essential condition for the design and optimization of fluid flow devices.

The paper is organized as follows. In Section 2, conservation equations of computational fluid dynamics, which represent the starting point of our analysis, are briefly summarized. In Section 3 the main results for the incompressible limit are reported, substantially supporting the basic assumption of the Thermodynamics of Irreversible Processes which assumes the Gibbs relation valid for non-equilibrium conditions as well. In Section 4 the main results for the compressible limit are reported. In Section 5 some consequences are derived from the previous results. Finally, in Section 6, the conclusions are reported.

2 Conservation equations of computational fluid dynamics

Let us consider the fundamental equations stipulating the balance of mass, momentum and total energy of the fluid [52,53], namely

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho\, \mathbf{u} \otimes \mathbf{u}) + \nabla p = \nabla \cdot \boldsymbol{\Pi}_\nu + \rho\, \mathbf{a}, \tag{2}$$

$$\frac{\partial (\rho e_t)}{\partial t} + \nabla \cdot (\rho e_t\, \mathbf{u} + p\, \mathbf{u}) = \nabla \cdot (-\mathbf{q} + \boldsymbol{\Pi}_\nu \cdot \mathbf{u}), \tag{3}$$

where ρ is the fluid density, $\mathbf{u}$ is the fluid velocity, p is the pressure, $\boldsymbol{\Pi}_\nu$ is the viscous part of the stress tensor, $\mathbf{a}$ is some spatially varying, external acceleration (e.g. the gravity), e_t is the total fluid energy per unit of mass and $\mathbf{q}$ is the thermal flux vector. Clearly the previous system of equations is not closed, and some phenomenological expressions are needed for $\boldsymbol{\Pi}_\nu$ and $\mathbf{q}$. Some popular expressions for Newtonian fluids are given by

$$\boldsymbol{\Pi}_\nu = \rho\nu \left[\nabla \mathbf{u} + \nabla \mathbf{u}^T - \frac{2}{3} (\nabla \cdot \mathbf{u})\, \mathbf{I} \right] + \rho\zeta\, (\nabla \cdot \mathbf{u})\, \mathbf{I}, \tag{4}$$

$$\mathbf{q} = -\lambda\, \nabla T, \tag{5}$$

where ν is the kinematic (shear) viscosity of the fluid, ζ is the bulk viscosity of the fluid and λ is the thermal conductivity. Eqs. (1, 2, 3), together with the phenomenological correlations (4) for $\boldsymbol{\Pi}_\nu$ and (5) for $\mathbf{q}$ represent the so-called Navier-Stokes-Fourier system of equations. The previous system of equations can be equivalently written in terms of Lagrangian total derivatives, namely $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$, as reported in A. The Lagrangian derivative is the fundamental operator ensuring Galilean invariance for the fluid dynamics (see B for details). Equations (1, 2, 3) are written in standard form (see A for details) and this allows one to say that mass and total energy are conserved, while momentum is conserved if and only if there is no external field, i.e. $\mathbf{a} = 0$. The physical meaning is that a conserved quantity can change its amount inside a fixed closed volume only by either accumulation inside

the same volume and/or fluxes at the border. Accumulation is described by the Eulerian time derivative ($\partial\varphi/\partial t$) and border effects by the divergence of fluxes ($\nabla\cdot\mathbf{f}(\varphi)$), according to the Gauss theorem.

The total energy is the sum of the mechanical energy e_m and the internal energy e_i, namely $e_t = e_m + e_i$. Let us derive first the equation for the mechanical energy e_m, defined as the sum of the kinetic energy $e_k = \mathbf{u}^2/2$ and the potential energy e_p such that $\mathbf{a} = -\nabla e_p$. Multiplying the Lagrangian form of (2) (see A for details) by $\mathbf{u}$ and recalling that $\mathbf{u}\cdot\nabla\mathbf{u}\cdot\mathbf{u} = \mathbf{u}\cdot\nabla e_k$, it follows

$$\rho\frac{\partial e_k}{\partial t} + \rho\mathbf{u}\cdot\nabla e_k - \rho\,\mathbf{u}\cdot\mathbf{a} = -(\nabla\cdot\boldsymbol{\Pi})\cdot\mathbf{u}, \tag{6}$$

where $\boldsymbol{\Pi} = p\,\mathbf{I} - \boldsymbol{\Pi}_\nu$ is the total stress tensor. Assuming that potential energy does not depend on time yields

$$\rho\frac{De_m}{Dt} = -(\nabla\cdot\boldsymbol{\Pi})\cdot\mathbf{u}, \tag{7}$$

and consequently

$$\rho\frac{De_m}{Dt} = -\nabla\cdot(\boldsymbol{\Pi}\cdot\mathbf{u}) + \boldsymbol{\Pi} : \nabla\mathbf{u}. \tag{8}$$

Coming back to standard form (see A for details) yields

$$\frac{\partial(\rho e_m)}{\partial t} + \nabla\cdot(\rho e_m\mathbf{u} + \boldsymbol{\Pi}\cdot\mathbf{u}) = \boldsymbol{\Pi} : \nabla\mathbf{u}, \tag{9}$$

where it is shown that mechanical energy is not conserved with the source (sink) term being at the right-hand side of (9).

¿From (9), it is straightforward to derive the equation for internal energy $e_i = e_t - e_m$, by subtraction with Eq. (3), namely

$$\frac{\partial(\rho e_i)}{\partial t} + \nabla\cdot(\rho e_i\,\mathbf{u} + \mathbf{q}) = -\boldsymbol{\Pi} : \nabla\mathbf{u}, \tag{10}$$

or equivalently, in Lagrangian form,

$$\rho\frac{De_i}{Dt} = -p\nabla\cdot\mathbf{u} - \nabla\cdot\mathbf{q} + \boldsymbol{\Pi}_\nu : \nabla\mathbf{u}. \tag{11}$$

We notice that internal energy is not conserved either, and the corresponding source/sink is equal in modulus (but with opposite sign) to the one for mechanical energy. The latter observation ensures that total energy, which is the sum of macroscopic (e_m) and microscopic (e_i) mechanical energies, is conserved instead. Finally, as typically done in the engineering community when dealing with open systems, we derive the expression for enthalpy h, defined as $h = e_i + pv$, where $v = 1/\rho$. Taking into account that

$$\rho\frac{Dh}{Dt} = \rho\frac{De_i}{Dt} + \frac{Dp}{Dt} - \frac{p}{\rho}\frac{D\rho}{Dt} = \rho\frac{De_i}{Dt} + \frac{Dp}{Dt} + p\nabla\cdot\mathbf{u}, \tag{12}$$

the equation for enthalpy can be derived by (11), namely

$$\rho\frac{Dh}{Dt} = -\nabla\cdot\mathbf{q} + \frac{Dp}{Dt} + \boldsymbol{\Pi}_\nu : \nabla\mathbf{u}, \tag{13}$$

or equivalently, in standard form,

$$\frac{\partial(\rho h)}{\partial t} + \nabla\cdot(\rho h\,\mathbf{u} + \mathbf{q}) = \frac{Dp}{Dt} + \boldsymbol{\Pi}_\nu : \nabla\mathbf{u}. \tag{14}$$

3 Results for the incompressible limit

The conservation equations of computational fluid dynamics can describe many different fluid flow regimes at the same time. On the other hand, different applications are interested usually in only few of them. For example, fluid dynamics of ground vehicles can be studied by the incompressible limit of Navier-Stokes-Fourier equations, while supersonic vehicles should be addressed with the compressible inviscid limit. These asymptotic limits can be rigorously defined by means of characteristic quantities. There are different ways to define characteristic quantities depending on what they refer to, i.e. fields or operators. Typically the magnitude of the velocity field is given by the characteristic quantity u_c, where $u_c = \max(\mathbf{u})$ on the considered domain. The same definition applies to the characteristic viscosity ν_c, namely $\nu_c = \max(\nu)$. Concerning operators, the definitions are slightly more difficult. For example, the characteristic time t_c and the characteristic length l_c are defined by

$$t_c = \frac{O(\varphi)}{O(\partial\varphi/\partial t)}, \tag{15}$$

$$l_c = \frac{O(\varphi)}{O(\nabla\varphi)} = \max_i\left(\frac{O(\varphi)}{O(\partial\varphi/\partial x_i)}\right), \tag{16}$$

respectively.

It is possible to use the previous characteristic quantities to define new operators. For example, in case of the Eulerian time derivative, it is possible to define $\partial/\partial\hat{t} = t_c\,\partial/\partial t$. From (15), it follows

$$t_c\,O(\partial\varphi/\partial t) = O(\partial\varphi/\partial\hat{t}) = O(\varphi). \tag{17}$$

The previous expression means that scaled operators (with "hat" notation), obtained by multiplying the original operator by the corresponding characteristic quantity, preserve the order of magnitude of the function they are applied to. Let us introduce the characteristic quantities and the scaled operators in Eq. (1), namely

$$\frac{l_c}{t_c\,u_c}\frac{\partial\rho}{\partial\hat{t}} + \hat{\nabla}\cdot(\rho\hat{\mathbf{u}}) = 0. \tag{18}$$

Introducing the Strouhal number $St = l_c/(t_c\,c_s)$ and the Mach number $Ma = u_c/c_s$, where c_s is the sound speed, yields

$$\frac{St}{Ma}\frac{\partial\rho}{\partial\hat{t}} + \hat{\nabla}\cdot(\rho\hat{\mathbf{u}}) = 0. \tag{19}$$

Similarly, we can proceed for the momentum equation (2), namely

$$\frac{u_c}{t_c}\frac{\partial(\rho\hat{\mathbf{u}})}{\partial\hat{t}} + \frac{u_c^2}{l_c}\hat{\nabla}\cdot(\rho\,\hat{\mathbf{u}}\otimes\hat{\mathbf{u}}) + \frac{1}{l_c}\hat{\nabla}p = \frac{u_c\,\nu_c}{l_c^2}\hat{\nabla}\cdot\hat{\boldsymbol{\Pi}}_\nu + \frac{u_c}{t_c}\rho\,\hat{\mathbf{a}}, \tag{20}$$

and consequently

$$St\,Ma\,\frac{\partial(\rho\hat{\mathbf{u}})}{\partial\hat{t}} + Ma^2\,\hat{\nabla}\cdot(\rho\,\hat{\mathbf{u}}\otimes\hat{\mathbf{u}}) + \frac{1}{c_s^2}\hat{\nabla}p = \\ = \frac{Ma^2}{Re}\hat{\nabla}\cdot\hat{\boldsymbol{\Pi}}_\nu + St\,Ma\,\rho\,\hat{\mathbf{a}}, \tag{21}$$

where $Re = u_c\,l_c/\nu_c$ is the Reynolds number.

We notice two issues in the latter expression: (a) There are multiple dimensionless numbers, i.e. St, Ma and Re defining the asymptotic regime; (b) One term is not properly scaled by them, i.e. $\hat{\nabla}p/c_s^2$. The first problem can be solved by selecting the Mach number as the asymptotic parameter, i.e. $Ma \ll 1$, and by specifying how all other dimensionless numbers scale with it. In particular, we set $t_c = l_c/u_c$ and hence $St = Ma$. Moreover, we assume that the Reynolds number is independent on Mach, i.e. $Re = O(1)$. These choices allow one to solve the second problem too: All terms in Eq. (21) become $O(Ma^2)$ and hence also the remaining term must have the same magnitude, i.e. $\hat{\nabla}p/c_s^2 = O(Ma^2)$. Consequently the pressure field can be split into two parts

$$\frac{p}{\rho_0\,c_s^2} = \gamma_p + Ma^2\,\hat{p}, \tag{22}$$

where ρ_0 is a proper constant depending on the initial conditions, γ_p is a dimensionless constant (which is not the heat capacity ratio) and $\hat{p}$ is the part dictating the fluid flow. The previous relation can be generalized to all thermodynamic quantities. Let us assume density ρ and temperature T as the two thermodynamic coordinates used to identify the thermodynamic state, namely $p = p(\rho, T)$. The previous equation highlights that the pressure field is characterized by small deviations from the constant $\gamma_p\,\rho_0\,c_s^2$, which can be expressed by the thermodynamic coordinates, namely

$$p = \gamma_p\,\rho_0\,c_s^2 + \left.\frac{\partial p}{\partial\rho}\right|_0(\rho-\rho_0) + \left.\frac{\partial p}{\partial T}\right|_0(T-T_0), \tag{23}$$

or equivalently

$$\left.\frac{\partial p}{\partial\rho}\right|_0(\rho-\rho_0) + \left.\frac{\partial p}{\partial T}\right|_0(T-T_0) = O(Ma^2). \tag{24}$$

Hence the largest possible deviations are given by

$$\frac{\rho}{\rho_0} = 1 + Ma^2\,\hat{\rho}, \tag{25}$$

$$\frac{T}{T_0} = 1 + Ma^2\,\hat{T}. \tag{26}$$

Substituting these new scalings into Eq. (19) yields

$$\hat{\nabla}\cdot\hat{\mathbf{u}} = O(Ma^2), \tag{27}$$

which is the fundamental relation for defining the incompressible limit of Navier-Stokes-Fourier system of equations.

¿From (27), it is possible to derive all other equations in the incompressible limit. Introducing the previous expressions into Eq. (21) yields

$$\frac{\partial(\rho\hat{\mathbf{u}})}{\partial\hat{t}} + \hat{\nabla}\cdot(\rho\,\hat{\mathbf{u}}\otimes\hat{\mathbf{u}}) + \hat{\nabla}\hat{p} = \frac{1}{Re}\hat{\nabla}\cdot\hat{\boldsymbol{\Pi}}_\nu + \rho\,\hat{\mathbf{a}}. \tag{28}$$

For the sake of simplicity, let us consider constant viscosity in the considered domain. In this case, the incompressible momentum equation becomes

$$\frac{\partial\hat{\mathbf{u}}}{\partial\hat{t}} + \hat{\mathbf{u}}\cdot\hat{\nabla}\hat{\mathbf{u}} + \frac{1}{\rho_0}\hat{\nabla}\hat{p} = \frac{1}{Re}\hat{\nabla}^2\hat{\mathbf{u}} + \hat{\mathbf{a}} + O(Ma^2). \tag{29}$$

Similarly, we can proceed with the enthalpy $h = h(\rho, T)$. Expanding the enthalpy around $\gamma_h\,c_s^2$, where γ_h is another dimensionless constant depending on the initial conditions, yields

$$h - \gamma_h\,c_s^2 = \left.\frac{\partial h}{\partial\rho}\right|_0(\rho-\rho_0) + \left.\frac{\partial h}{\partial T}\right|_0(T-T_0). \tag{30}$$

Taking into account Eqs. (25, 26), the scaling for enthalpy follows, namely

$$\frac{h}{c_s^2} = \gamma_h + Ma^2\,\hat{h}. \tag{31}$$

Introducing the previous characteristic quantities and scaled operators in Eq. (13) yields

$$\rho\frac{1}{c_s^2}\frac{\hat{D}h}{D\hat{t}} = -\frac{\rho_0\,\gamma_0\,Ma^2}{Pr\,Re}\hat{\nabla}\cdot\hat{\mathbf{q}}_\alpha + \frac{1}{c_s^2}\frac{\hat{D}p}{D\hat{t}} + \frac{Ma^2}{Re}\hat{\boldsymbol{\Pi}}_\nu : \hat{\nabla}\hat{\mathbf{u}}, \tag{32}$$

where $Pr = \nu_c/\alpha_c$ is the Prandtl number, $\alpha_c = \lambda_c/(\rho_0\,c_0)$ is the thermal diffusivity, c_0 is the specific heat capacity and $\gamma_0 = c_0\,T_0/c_s^2$ is a constant. Introducing the scaling relations given by Eqs. (31, 22) into the previous equation yields

$$\rho\,\frac{\hat{D}\hat{h}}{D\hat{t}} = -\frac{\rho_0\,\gamma_0}{Pr\,Re}\hat{\nabla}\cdot\hat{\mathbf{q}}_\alpha + \frac{\hat{D}\hat{p}}{D\hat{t}} + \frac{1}{Re}\hat{\boldsymbol{\Pi}}_\nu : \hat{\nabla}\hat{\mathbf{u}}, \tag{33}$$

and consequently, taking into account all previous asymptotic results (in particular Eq. (27)), the enthalpy equation for incompressible flows reads

$$\frac{\hat{D}\hat{h}}{D\hat{t}} = -\frac{\gamma_0}{Pr\,Re}\hat{\nabla}\cdot\hat{\mathbf{q}}_\alpha + \frac{1}{\rho_0}\frac{\hat{D}\hat{p}}{D\hat{t}} + \dots \\ \dots + \frac{1}{Re}(\hat{\nabla}\hat{\mathbf{u}} + \hat{\nabla}\hat{\mathbf{u}}^T) : \hat{\nabla}\hat{\mathbf{u}} + O(Ma^2). \tag{34}$$

It is possible to simplify the notations in (34) by focusing on the notion of strain rate, as shown below. Let us introduce the strain rate tensor $\nabla^S\mathbf{u} = (\nabla\mathbf{u} + \nabla\mathbf{u}^T)/2$ and the vorticity tensor $\nabla^W\mathbf{u} = (\nabla\mathbf{u} - \nabla\mathbf{u}^T)/2$. It is easy to prove that $\nabla\mathbf{u} = \nabla^S\mathbf{u} + \nabla^W\mathbf{u}$ and, more importantly, $\nabla^S\mathbf{u} : \nabla^W\mathbf{u} = 0$. Making use of these definitions in the previous expression yields

$$\frac{\hat{D}\hat{h}}{D\hat{t}} = -\frac{\gamma_0}{Pr\,Re}\hat{\nabla}\cdot\hat{\mathbf{q}}_\alpha + \frac{1}{\rho_0}\frac{\hat{D}\hat{p}}{D\hat{t}} + \frac{2}{Re}(\hat{\nabla}^S\hat{\mathbf{u}})^2 + O(Ma^2), \tag{35}$$

where $(\hat{\nabla}^S\hat{\mathbf{u}})^2 = \hat{\nabla}^S\hat{\mathbf{u}} : \hat{\nabla}^S\hat{\mathbf{u}}$. For the sake of simplicity, let us consider constant thermal conductivity in the considered domain, namely

$$\frac{\hat{D}\hat{h}}{D\hat{t}} = \frac{\gamma_0}{Pr\,Re}\hat{\nabla}^2\hat{T} + \frac{1}{\rho_0}\frac{\hat{D}\hat{p}}{D\hat{t}} + \frac{2}{Re}(\hat{\nabla}^S\hat{\mathbf{u}})^2 + O(Ma^2). \quad (36)$$

In the asymptotic limit $Ma \to 0$, coming back to physical units assuming constant thermo-physical properties for the sake of simplicity, the incompressible limit of the Navier-Stokes-Fourier system of equations can be written as

$$\nabla \cdot \mathbf{u} = 0, \quad (37)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\frac{1}{\rho_0}\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{a}, \quad (38)$$

$$\frac{\partial h}{\partial t} + \mathbf{u}\cdot\nabla h = \frac{\lambda}{\rho_0}\nabla^2 T + 2\nu(\nabla^S\mathbf{u})^2 + \frac{1}{\rho_0}\frac{Dp}{Dt}. \quad (39)$$

Towards an effort of exploring the (slightly) non-equilibrium thermodynamics of the incompressible limit, it is essential to derive an equation for entropy and, in particular, for entropy production. Let us follow the guidelines of the Thermodynamics of Irreversible Processes (TIP) [43,44]. The key idea is to assume that local equilibrium holds, i.e. all subparts of the system are close enough to equilibrium condition to be still described by classical thermodynamic variables and relationships. In a state of thermodynamic equilibrium, there is a fundamental relation (Gibbs relation) which provides the connection between entropy and other thermodynamic potentials, namely $Tds = de_i + pdv$. The first simple (but powerful) idea is to assume that the same relation holds in non-equilibrium conditions as well. In non-equilibrium states, the previous expression becomes the definition of entropy. Of course, this definition must be Galilean invariant and hence Lagrangian time derivatives must be considered for this goal (see B for details), namely

$$T\frac{Ds}{Dt} = \frac{De_i}{Dt} + p\frac{Dv}{Dt} = \frac{Dh}{Dt} - v\frac{Dp}{Dt}, \quad (40)$$

or equivalently

$$\rho T\frac{Ds}{Dt} = \rho\frac{Dh}{Dt} - \frac{Dp}{Dt}. \quad (41)$$

Substituting Eq. (13) into Eq. (41) yields

$$\rho T\frac{Ds}{Dt} = -\nabla\cdot\mathbf{q} + 2\,\rho\nu\,(\nabla^S\mathbf{u})^2 + \rho\left(\zeta - \frac{2}{3}\nu\right)(\nabla\cdot\mathbf{u})^2. \quad (42)$$

In the incompressible limit, namely at very low Mach number flows, according to Eq. (37), the last term of the previous expression can be neglected. Taking into account the definition of thermal flux according to Fourier's law given by Eq. (5) and assuming constant thermo-physical properties for the sake of simplicity yield

$$\rho\frac{Ds}{Dt} = \frac{\lambda}{T}\nabla^2 T + \frac{2\,\mu}{T}(\nabla^S\mathbf{u})^2, \quad (43)$$

where $\mu = \rho\,\nu$ is the dynamic viscosity. Elaborating further on the first term at the right hand side of the previous expression yields

$$\rho\frac{Ds}{Dt} + \nabla\cdot\left(\frac{1}{T}\,\mathbf{q}\right) = \frac{\lambda}{T^2}(\nabla T)^2 + \frac{2\,\mu}{T}(\nabla^S\mathbf{u})^2 \geq 0. \quad (44)$$

Taking into account the general property given by Eq. (59), the previous equation can be rewritten in standard form, namely

$$\frac{\partial(\rho s)}{\partial t} + \nabla\cdot\mathbf{f}(\rho s) = \sigma_\alpha + \sigma_\nu \geq 0, \quad (45)$$

where

$$\mathbf{f}(\rho s) = \rho s\,\mathbf{u} + \frac{1}{T}\,\mathbf{q} = \rho s\,\mathbf{u} + k_B\,\beta\,\mathbf{q}, \quad (46)$$

k_B is the Boltzmann constant, $\beta = 1/(k_B\,T)$ (as common in statistical mechanics) and the entropy production terms are defined by

$$\sigma_\alpha = \rho\,\alpha\left(\frac{c_0}{T^2}\right)(\nabla T)^2 \geq 0, \quad (47)$$

$$\sigma_\nu = \rho\,\nu\left(\frac{2}{T}\right)(\nabla^S\mathbf{u})^2 \geq 0. \quad (48)$$

Each entropy production term describes the entropy produced by a specific transport phenomenon: σ_α takes into account the entropy produced by heat transfer, which is ruled by temperature gradient, and σ_ν the entropy produced by fluid flow, which is ruled by strain rate. Clearly each entropy production mechanism satisfies the second law of thermodynamics, namely $\sigma_\alpha \geq 0$ and $\sigma_\nu \geq 0$, and so it does the global entropy production, namely $\sigma_\alpha + \sigma_\nu \geq 0$. This confirms the validity of the assumption given by Eq. (40) for non-equilibrium states in the incompressible limit.

4 Results for the compressible limit

In the generic compressible case, the situation is slightly more complex. Let us rewrite Eq. (42) as follows

$$\rho T\frac{Ds}{Dt} = -\nabla\cdot\mathbf{q} + 2\,\rho\nu\left[(\nabla^S\mathbf{u})^2 - \frac{1}{3}(\nabla\cdot\mathbf{u})^2\right] + \ldots$$
$$\ldots + \rho\zeta\,(\nabla\cdot\mathbf{u})^2. \quad (49)$$

Following Ref. [44], let us consider the following equivalence

$$(\nabla^S\mathbf{u})^2 - \frac{1}{3}(\nabla\cdot\mathbf{u})^2 = (\nabla^S\mathbf{u})^2 + \frac{1}{3}(\nabla\cdot\mathbf{u})^2 + \ldots$$
$$\ldots - \frac{2}{3}(\nabla\cdot\mathbf{u})^2 = \nabla^S\mathbf{u} : \nabla^S\mathbf{u} + \frac{1}{9}(\nabla\cdot\mathbf{u})^2\,\mathbf{I}:\mathbf{I} + \ldots$$
$$\ldots - \frac{1}{3}(\nabla\cdot\mathbf{u})\,\mathbf{I} : \nabla^S\mathbf{u} - \frac{1}{3}(\nabla\cdot\mathbf{u})\,\nabla^S\mathbf{u} : \mathbf{I} =$$
$$= \left[\nabla^S\mathbf{u} - \frac{1}{3}(\nabla\cdot\mathbf{u})\,\mathbf{I}\right]^2, \quad (50)$$

where the property $\mathbf{I} : \mathbf{I} = 3$ was used. Using the equivalence given by Eq. (50) in Eq. (49) and proceeding as before, the final entropy balance equation, which is valid for any fluid dynamic regimes, becomes

$$\frac{\partial(\rho s)}{\partial t} + \nabla \cdot \mathbf{f}(\rho s) = \sigma_\alpha + \sigma'_\nu + \sigma_\zeta = \sigma \geq 0, \tag{51}$$

where

$$\sigma_\alpha = \rho\,\alpha \left(\frac{c_0}{T^2}\right) (\nabla T)^2 \geq 0, \tag{52}$$

$$\sigma'_\nu = \rho\,\nu \left(\frac{2}{T}\right) \left[\nabla^S \mathbf{u} - \frac{1}{3}(\nabla \cdot \mathbf{u})\,\mathbf{I}\right]^2 \geq 0, \tag{53}$$

$$\sigma_\zeta = \rho\,\zeta \left(\frac{1}{T}\right) (\nabla \cdot \mathbf{u})^2 \geq 0. \tag{54}$$

The previous derivation allows one to identify the generalized thermodynamic forces, as discussed in the following section.

5 Discussion

Equation (45), as a consequence of the assumption (40), confirms the applicability of the Thermodynamics of Irreversible Processes to incompressible flows. Moreover, assumption (40) is also valid for compressible flows, as far as the entropy production σ'_ν given by Eq. (53) is used instead of σ_ν given by Eq. (48).

1. Equation (45) extends the original expressions for entropy balance to fluid flow (see Refs. [43,44] for mass diffusion) by the assumption (40), which is the simplest possible extension of the fundamental thermodynamics relation $Tds = de_i + pdv$ to non-equilibrium fluid flows.
2. In case of highly compressible flows, there are three terms which are responsible of the entropy production, as reported in Eq. (51): in addition to σ_α in (47) and σ'_ν in (53), which is the generalization of the former σ_ν, a novel term σ_ζ is derived in (54), which is proportional to the bulk viscosity of the fluid. All these terms (and consequently their sum) are consistent with the second law of thermodynamics (i.e. positively defined).
3. The entropy production in Eq. (51) can be rewritten as

   $$\sigma = \sum_k \eta_k\, X_k^2, \tag{55}$$

   where η_k are the phenomenological coefficients of the irreversible phenomena (in particular, $\eta_0 = \rho\zeta/T$, $\eta_1 = \rho\alpha\, c_0/T^2$ and $\eta_2 = \rho\nu\, 2/T$) and X_k the generalized thermodynamic forces ($X_0 = \nabla \cdot \mathbf{u}$, $X_1 = \nabla T$ and $X_2 = \nabla^S \mathbf{u} - (\nabla \cdot \mathbf{u}/3)\,\mathbf{I}$). The subscript k has been selected equal to the dimensionality of the corresponding thermodynamic force (scalar $k = 0$, vector $k = 1$, tensor $k = 2$). Consequently $X_k^2 = X_k * X_k$ where the generalized product $*$ means simple product for $k = 0$, scalar product $\cdot$ for $k = 1$ and saturation product : for $k = 2$. Equation (55) can be further rewritten as

   $$\sigma = \sum_k J_k * X_k, \tag{56}$$

   where $J_k = \eta_k\, X_k$ is the generalized thermodynamic flux. For the sake of simplicity, in this work, we considered $J_k = \eta_k\, X_k$, which only takes into account the diagonal terms of the more general expression $J_k = \sum_l L_{kl} X_l$ with L_{kl} being the Onsager's matrix of phenomenological coefficients. Hence, our derivation is also consistent with the general formalism of linear irreversible processes in non-equilibrium thermodynamics. However, it is worth the effort to point out that, in the case of compressible flows, the same intensive quantity $\mathbf{u}$ is generating two generalized forces, namely $X_0 = \nabla \cdot \mathbf{u}$ and $X_2 = \nabla^S \mathbf{u} - (\nabla \cdot \mathbf{u}/3)\,\mathbf{I}$. Hence the corresponding entropy production must be described by two phenomenological coefficients, namely $\eta_0 = \rho\zeta/T$ and $\eta_2 = \rho\nu\, 2/T$. This is definitively not surprising, taking into account the dimensionality of the intensive quantity $\mathbf{u}$ in comparison with other scalar quantity $1/T$.

6 Conclusions

In the present paper, we aim to present an overview of the entropy production in fluid dynamics in a more systematic way. First of all, we clarify the rigorous derivation of the incompressible limit of Navier-Stokes-Fourier system of equations by means of the asymptotic analysis, which is a very well known mathematical technique used to derive macroscopic limits of kinetic equations. This allows to overcome the theoretical limits of assuming that the material derivative of the density simply vanishes.

Secondly, we show how the fundamental Gibbs relation in classical thermodynamics can be applied to non-equilibrium flows for generalizing the concept of entropy and hence the second law of thermodynamics for both incompressible and compressible flows. This is consistent with the Thermodynamics of Irreversible Processes (TIP). The second law of thermodynamics given by Eq. (51) is an essential condition for the design and optimization of fluid flow devices (e.g. by the entropy generation minimization approach [55,56]).

Providing an overview of the theoretical framework for irreversibilities, consistently valid at different regimes

(both incompressible and compressible), sheds light on entropy production in fluid mechanics, with broad implications in applied mechanics.

A Lagrangian formulation

Conservation equations in computational fluid dynamics can be conveniently written in standard form, namely

$$\frac{\partial \varphi}{\partial t} + \nabla \cdot \mathbf{f}(\varphi) = s(\varphi), \tag{57}$$

where φ is a generic quantity (density, momentum, total energy, mechanical energy, kinetic energy, internal energy, entropy, etc.), $\mathbf{f}(\varphi)$ is the corresponding flux and $s(\varphi)$ the corresponding source/sink.

If a quantity has a balance equation written in standard form such that $s(\varphi) = 0$, then this quantity is conserved and the corresponding equation is a conservation equation. The physical meaning is that a conserved quantity changes inside a fixed closed volume only by accumulation inside the same volume and/or fluxes at the border. Accumulation is described by the Eulerian time derivative ($\partial\varphi/\partial t$) and border effects by the divergence of fluxes ($\nabla \cdot \mathbf{f}(\varphi)$), according to the Gauss theorem.

There is also another useful form for conservation equations, which involves the Lagrangian derivative $D\varphi/Dt$, namely

$$\frac{D\varphi}{Dt} \doteq \frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi. \tag{58}$$

The Lagrangian time derivative is Galilean invariant (see B for details) and this ensures that it has the same values in all inertial frames. Taking into account the mass conservation equation (1), the following property holds

$$\frac{\partial(\rho\varphi)}{\partial t} + \nabla \cdot (\rho\varphi\mathbf{u}) = \rho\frac{\partial \varphi}{\partial t} + \rho\mathbf{u} \cdot \nabla\varphi \ldots$$
$$\ldots + \varphi\frac{\partial \rho}{\partial t} + \varphi\nabla \cdot (\rho\mathbf{u}) = \rho\frac{D\varphi}{Dt}. \tag{59}$$

Consequently the Lagrangian formulation of the Navier-Stokes-Fourier system of equations is given by

$$\frac{D\rho}{Dt} = -\rho\nabla \cdot \mathbf{u}, \tag{60a}$$
$$\rho\frac{D\mathbf{u}}{Dt} = -\nabla \cdot \boldsymbol{\Pi} + \rho\,\mathbf{a}, \tag{60b}$$
$$\rho\frac{De_t}{Dt} = -\nabla \cdot (\mathbf{q} + \boldsymbol{\Pi} \cdot \mathbf{u}). \tag{60c}$$

From the previous expressions, it is easy to prove that the Navier-Stokes-Fourier system of equations is Galilean invariant.

B Galilean invariance

Galilean invariance states that the laws of motion are the same in all inertial frames. Galileo Galilei first described this principle in 1632. In non-relativistic mechanics, it is possible to introduce a Galilean transformation in order to verify if an operator is Galilean invariant, namely

$$\begin{cases} t^* = t, \\ \mathbf{x}^* = \mathbf{x} - \mathbf{c}\,t, \\ \mathbf{u}^* = \mathbf{u} - \mathbf{c}, \end{cases} \tag{61}$$

where t, $\mathbf{x}$, $\mathbf{u}$ are time, position vector and velocity vector in the reference frame assumed at rest, t^*, $\mathbf{x}^*$, $\mathbf{u}^*$ are time, position vector and velocity vector in the moving frame and $\mathbf{c}$ is the velocity of the moving frame (with respect to the rest one). Once the quantities in the frame at rest are known, the previous transformation allows one to compute the corresponding quantities in the moving frame. An operator is said to be Galilean invariant if and only if it is invariant with regards to the application of the previous transformation.

Let us consider the Lagrangian time derivative (see Eq. (58) in A). The generic quantity φ is measured first in the frame at rest and hence it can be considered a function of t and $\mathbf{x}$, namely $\varphi = \varphi(t, \mathbf{x})$. However, by means of the transformation given by Eqs. (61), t and $\mathbf{x}$ themselves can be considered as functions of the quantities in the moving frame by parameter $\mathbf{c}$, namely $t = t(t^*, \mathbf{x}^*, \mathbf{u}^*; \mathbf{c})$ and $\mathbf{x} = \mathbf{x}(t^*, \mathbf{x}^*, \mathbf{u}^*; \mathbf{c})$. Consequently also $\varphi = \varphi(t^*, \mathbf{x}^*; \mathbf{c})$ holds. When computing the derivative of $\varphi = \varphi(t^*, \mathbf{x}^*; \mathbf{c})$ with regards to D/Dt expressed in the frame at rest, some mixed derivatives appear which can be solved by the chain rule, namely

$$\frac{D\varphi}{Dt} = \frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla\varphi = \frac{D\varphi(t^*, \mathbf{x}^*)}{Dt} =$$
$$= \frac{\partial \varphi}{\partial t^*}\frac{\partial t^*}{\partial t} + \nabla^*\varphi \cdot \frac{\partial \mathbf{x}^*}{\partial t} + (\mathbf{u}^* + \mathbf{c}) \cdot \left(\frac{\partial \varphi}{\partial t^*}\nabla t^* + \nabla^*\varphi \cdot \nabla\mathbf{x}^*\right) =$$
$$= \frac{\partial \varphi}{\partial t^*} + \nabla^*\varphi \cdot (-\mathbf{c}) + (\mathbf{u}^* + \mathbf{c}) \cdot \nabla^*\varphi = \frac{D^*\varphi}{Dt^*}. \tag{62}$$

The latter expression proves that the value of the Lagrangian time derivative is the same if computed in any inertial frame and hence it is Galilean invariant.

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